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TWO-BODY COLLISIONS AND MEAN-FIELD THEORY: THE BRUECKNER–BOLTZMANN EQUATION

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Starting from the BBGKY hierarchy of density matrices, a quantum mechanical Boltzmann equation, including a mean field, is derived. Both the mean field, which is of the well-known Brueckner–Hartree–Fock form, as well as the collision term are expressed in terms of the self-consistent Brueckner G-matrix. The relation with the generalized Boltzmann equation of Kadanoff and Baym is discussed. It is shown that the usual quantum mechanical theories like TDHF and Uehling–Uhlenbeck appear as limiting cases.

To describe nuclear reactions in the intermediate energy domain, one requires a quantum mechanical kinetic equation which comprises in a consistent way both a mean-field and a two-body collision term. Many attempts to derive such an equation are recorded in the literature. Some are formulated as an extension of the TDHF theory [1–5] and consequently have the same drawbacks, namely the unavoidable use of a phenomenological effective interaction like the Skyrme forces and the problem of incorporating dissipative i.e. irreversible aspects. Others are very general and therefore pose practical problems as to their solution [6,7]. Furthermore the use of the Green function formalism complicates things considerably. In contrast there exists a nice approach due to Snider [8], based on density matrices, which has the required physical transparency. While Snider used this formalism to derive a quantum mechanical Boltzmann equation for the case of a dilute gas, we will use it to derive a quantum kinetic equation which applies to medium- and high-energy nuclear reactions. In doing this we use the self-consistent Brueckner–Bethe–Goldstone method to describe nuclear interactions.

The time evolution of a N-particle system is determined by the Liouville–von Neumann equation for the N-particle density matrix ρ:

$$i\hbar\,\partial_t \rho = [H, \rho]\ , \tag{1}$$

where H is the total N-particle hamiltonian, here taken to be

$$H = \sum_{i=1}^{N} K_i + \sum_{i<j=1}^{N} V_{ij}\ . \tag{2}$$

In order to get the BBGKY hierarchy, one introduces reduced (n)-particle density matrices as follows:

$$\rho^{(n)}_{12\ldots n} = \frac{N!}{(N-n)!}\ \mathop{\mathrm{Tr}}_{(n+1\ldots N)}\ \rho\ ,$$

$$\mathop{\mathrm{Tr}}_{(1\ldots n)}\ \rho^{(n)}_{12\ldots n} = \frac{N!}{(N-n)!}\ , \tag{3}$$

and by taking the appropriate traces in eq. (1), one gets

$$i\hbar\,\partial_t \rho^{(n)}_{12\ldots n} = \sum_{i=1}^{n} [K_i, \rho^{(n)}_{12\ldots n}] + \sum_{i<j=1}^{n} [V_{ij}, \rho^{(n)}_{12\ldots n}]$$

$$+ \mathop{\mathrm{Tr}}_{(n+1)} \sum_{i=1}^{n} [V_{i\,n+1}, \rho^{(n+1)}_{12\ldots n+1}]\ . \tag{4}$$

This set of equations is equivalent to eq. (1).

Using the simplified notation: $\rho_i \equiv \rho_i^{(1)}$; $\rho_{ij} \equiv \rho_{ij}^{(2)}$, etc., the first two members of the hierarchy read

$$i\hbar\,\partial_t \rho_1 = [K_1, \rho_1] + \mathop{\mathrm{Tr}}_{(2)} [V_{12}, \rho_{12}] \tag{5}$$

$$i\hbar\partial_t \rho_{12} = [K_1 + K_2 + V_{12}, \rho_{12}]$$

$$+ \operatorname{Tr}_{(3)} [V_{13} + V_{23}, \rho_{123}]. \quad (6)$$

To solve eq. (5) for ρ_1, we have to express the two-particle density matrix ρ_{12} as a functional of one-particle density matrices. The most simple way to do this, is by neglecting all two-particle correlations except the ones imposed by the identity of the particles through antisymmetrisation:

$$\rho_{12} = \rho_1 \rho_2 A_{12} \quad (A_{ij} = 1 - P_{ij}), \quad (7)$$

where A_{ij} is the antisymmetrisation operator for fermions and P_{ij} denotes the permutation operator. Using expression (7) in eq. (5) results in the TDHF equation for ρ_1.

However, to obtain a Boltzmann-like equation, two-particle correlations have to be taken into account and expressed in terms of one-body entities. Snider [8] attained this for the case of a dilute gas with short-range binary interactions only. In that case, one particle feels at the most the interaction with one other particle and therefore the trace term in eq. (6) can be set to zero, and the equation for ρ_{12} can be solved, given an initial condition. Since it follows from the assumptions that the average time between collisions is much longer than the collision time (weak-coupling limit), we can take ρ_{12} to be uncorrelated before the actual collision and at these times it can be expressed in ρ_i like in eq. (7). With this initial condition the solution for ρ_{12} reads

$$\rho_{12} = \Omega_{12} \rho_1 \rho_2 A_{12} \Omega_{12}^\dagger, \quad (8)$$

with

$$\Omega_{12} = \lim_{\tau \to -\infty} \exp[(i/\hbar)(K_1 + K_2 + V_{12})\tau]$$

$$\times \exp[-(i/\hbar)(K_1 + K_2)\tau] \quad (9)$$

the usual Møller operator from scattering theory [9], which can be expressed in terms of the T-matrix. The resulting equation for ρ_1 has all the features of a Boltzmann equation and is known as the Waldmann–Snider equation [8,10]. From it one can obtain the Uehling–Uhlenbeck eq. (11) as a special case. Note that if we set the interaction V_{12} in (9) equal to zero, the Møller operator becomes the unity operator and we regain the TDHF form for ρ_{12} (eq. (7)).

We will now apply the same techniques to the nuclear case. In contrast with the case of a dilute gas we may not simply neglect three-body correlations. Instead we will handle them by a well-known method in nuclear matter theory, the Brueckner–Bethe–Goldstone method. In doing this, we will make explicit use of form (8) and in fact only try to find the proper expression for Ω, which must now incorporate the just mentioned many-body effects.

In the Brueckner–Bethe–Goldstone approach, two particles interact with each other while each of them moves independently in a mean field generated by the effective interactions with all the other particles. This results in a very specific form for the three-particle correlation term in eq. (6) for ρ_{123}:

$$\rho_{123} = \Omega_{13} \rho_{12} \rho_3 A_{13} \Omega_{13}^\dagger + \Omega_{23} \rho_{12} \rho_3 A_{23} \Omega_{23}^\dagger, \quad (10)$$

and amounts to a first-order approximation to the full three-particle Møller operator Ω_{123} for ρ_{123} [12], as can be understood by inspecting the Faddeev equations for three-particle scattering [9]. The second step consists of evaluating the trace term in eq. (6). By using a general property of Møller operators [9]: $\Omega = 1 + gV\Omega$, where g denotes the Green function, we can separate mean-field and higher-order effects. This can be done by retaining only the terms linear in either Ω_{13} or Ω_{23}:

$$\operatorname{Tr}_{(3)} [V_{13} + V_{23}, \rho_{123}]$$

$$\simeq \operatorname{Tr}_{(3)} |[V_{13}\Omega_{13}A_{13}\rho_3 + V_{23}\Omega_{23}A_{23}\rho_3, \rho_{12}]|$$

$$= |[U_1 + U_2, \rho_{12}]|, \quad (11)$$

where the commutator with the double bar is defined as

$$|[A, B]| \equiv AB - BA^\dagger, \quad (12)$$

and

$$U_i \equiv \operatorname{Tr}_{(3)} V_{i3} \Omega_{i3} A_{i3} \rho_3 \quad (i = 1, 2), \quad (13)$$

which is the mean-field contribution. With the approximation given in eq. (11) we achieved that indeed particles 1 and 2, while interacting by means of the potential V_{12}, propagate independently in their re-

spective mean fields U_1 and U_2, as can be seen from the resulting equation for ρ_{12}:

$$i\hbar\partial_t\rho_{12} = |[K_1 + K_2 + V_{12} + U_1 + U_2, \rho_{12}]|. \quad (14)$$

Solving this equation will result in an expression for Ω_{12} by virtue of it defining relation (8). Since U_i itself depend on this solution (eq. (13)) self-consistency is built-in. The formal solution of eq. (14) can be written as

$$\rho_{12}(t) = \underset{\leftarrow}{\mathrm{T}} \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt' |[K_1 + K_2 + V_{12} + U_1(t') + U_2(t'), \quad]|\right)\rho_{12}(t_0), \quad (15)$$

where T is the time-ordering operator and where the arrow denotes the direction of the time-ordering of the operators U_i.

In general, at time t, the particles will be interacting, i.e. they are correlated. Assuming the weak-coupling limit where the average time between collisions is much longer than the collision time it is possible to find an earlier time t_0 before the collision at which the particles are uncorrelated:

$$\rho_{12}(t_0) = \rho_1(t_0)\rho_2(t_0)A_{12}. \quad (16)$$

Since at a fixed t_0 and on a microscopic time scale some of the particles might be uncorrelated, others however, are in the middle of a collision. Therefore (16) is only correct if interpreted as coarse-grained density matrices [13], i.e. time-averaged over an interval which is of the order of the collision time t_{coll} but smaller than the mean free time t_{m} in between collisions. This coarse-graining implies that we regard the microscopic details on time scales t_{coll} as irrelevant for the statistical evolution of the system. Before a collision the memory about dynamical correlations from previous collisions is wiped out (markovian process). This is fully equivalent to Boltzmann's assumption of molecular chaos (stosszahlansatz) and because it introduces a distinction between the event "before the collision" and the event "after a collision" it is the very origin of irreversibility.

Concerning the applicability of the weak-coupling limit to nucleus–nucleus collisions we restrict ourselves here to reactions where the bombarding energy per nucleon exceeds the Fermi energy (i.e. 30 MeV/nucleon). The collision time is estimated as

$$t_{\mathrm{coll}} \simeq (2/v)\,\mathrm{d}\delta/\mathrm{d}k \simeq 2a/v',$$

with v the velocity and δ the ($l = 0$) phase shift which for a hard core of radius a has the value $-ka$. The mean free time $t_{\mathrm{m}} \simeq 1/\rho\bar{\sigma}$ with ρ the (local) density and $\bar{\sigma}$ the effective (medium-corrected) nucleon–nucleon cross section. The latter was calculated in ref. [14] and it was found that $\bar{\sigma} \leqslant 20$ mb. Therefore we have $t_{\mathrm{m}} > t_{\mathrm{coll}}$ and this suggests that in this energy domain the weak-coupling limit is reasonably fulfilled.

Expression (16) enables us to express the pair density matrix in terms of the one-particle density matrix. By consistently applying in eq. (5) the same linearisation procedure (i.e. relation (11)):

$$\begin{aligned}\underset{(2)}{\mathrm{Tr}}\,[V_{12}, \rho_{12}] &= \underset{(2)}{\mathrm{Tr}}\,[V_{12}, \Omega_{12}\rho_1\rho_2 A_{12}\Omega_{12}^{\dagger}] \\ &\simeq \underset{(2)}{\mathrm{Tr}}\,|[V_{12}\Omega_{12}A_{12}\rho_2, \rho_1]| \\ &= |[U_1, \rho_1]|, \end{aligned} \quad (17)$$

we can transform the uncorrelated pair back from t_0 to t in an uncorrelated way:

$$\rho_1(t_0)\,\rho_2(t_0) = \underset{\rightarrow}{\mathrm{T}} \exp\left(\frac{i}{\hbar}\int_{t_0}^{t} dt' |[K_1 + K_2 + U_1(t') + U_2(t'), \quad]|\right)\rho_1(t)\,\rho_2(t). \quad (18)$$

Combining eqs. (8), (15), (16) and (18), we find

$$\begin{aligned}\Omega_{12}(t) = \underset{\leftarrow}{\mathrm{T}} \exp\Big(-\frac{i}{\hbar}\int_{t_0}^{t} dt' [K_1 + K_2 + V_{12} + U_1(t') + U_2(t')]\Big) \\ \times \underset{\rightarrow}{\mathrm{T}} \exp\left(\frac{i}{\hbar}\int_{t_0}^{t} dt' [K_1 + K_2 + U_1(t') + U_2(t')]\right), \end{aligned} \quad (19)$$

where we used the operator identity

$$\exp[(i/\hbar)|[A,]|]B = \exp[(i/\hbar)A]B\exp[-(i/\hbar)A^{\dagger}].$$

Because the time difference between t and t_0 is of the order of t_{coll}, the mean field will only slightly change and we can write

$$\int_{t_0}^{t} \mathrm{d}t' \, U_i(t') \simeq U_i(t)(t - t_0) . \tag{20}$$

The time t_0 is "long" before the particles collide which means long compared to the duration of a collision t_{coll} but short compared to the time between collisions t_{m}. The total interaction so to speak has been "split up" in a hard part (inducing correlations, through the Ω_{12} operator) of a short duration t_{coll} and a soft smooth part (no correlations, through the mean field U_i) during t_{m}. Thus from a collision point of view, the mathematical limit $t_0 \to -\infty$ can be taken although macroscopically t_0 must be small. This separation of time scales is to be implicitly assumed when the limit $t_0 \to -\infty$ is taken.

By using (20) and taking the mathematical limit $t_0 \to -\infty$ in eq. (19) we obtain

$$\begin{aligned}\Omega_{12}(t) = \lim_{\tau \to \infty} & \exp\{-(\mathrm{i}/\hbar)[K_1 + K_2 + V_{12} \\ & + U_1(t) + U_2(t)]\tau\} \\ & \times \exp\{(\mathrm{i}/\hbar)[K_1 + K_2 + U_1(t) + U_2(t)]\tau\} \\ & \equiv \lim_{\tau \to \infty} \exp[(\mathrm{i}/\hbar) H_{12}(t)\tau] \exp[-(\mathrm{i}/\hbar) H_{12}^{(0)}(t)\tau] ,\end{aligned} \tag{21}$$

which, except for the time-dependent mean fields, is the usual Møller operator (eq. (9)). The hamiltonians $H_{12}(t)$ and $H_{12}^{(0)}(t)$, respectively, play the role of the total and the unperturbed one. If $H_{12}(t)$ and $H_{12}^{(0)}(t)$ have complete sets of eigenstates corresponding to the same eigenvalue $E_{12}(t)$, we can apply conventional scattering theory and as a result we get

$$\Omega_{12}(t) = 1 + \frac{Q_{12}(t)}{E_{12}(t) - H_{12}^{(0)}(t) + \mathrm{i}\epsilon} V_{12}\Omega_{12}(t) , \tag{22}$$

with $Q_{12}(t)$ the time-dependent Pauli projection operator, which in the Goldstone representation (neglecting hole–hole scattering) can be written as

$$Q_{12}(t) = [1 - \rho_1(t)][1 - \rho_2(t)] . \tag{23}$$

By defining a time-dependent Brueckner G-matrix

$$G_{12}(t) = V_{12}\Omega_{12}(t) , \tag{24}$$

the well-known equation for the G-matrix follows:

$$G_{12}(t) = V_{12} + \frac{Q_{12}(t)}{E_{12}(t) - H_{12}^{(0)}(t) + \mathrm{i}\epsilon} G_{12}(t) . \tag{25}$$

Putting everything together, i.e. eq. (8), (22) and (24) into eq. (5), we finally arrive at what we call the Brueckner–Boltzmann equation in operator form:

$$\begin{aligned}\mathrm{i}\hbar\partial_t \rho_1 = & [K_1, \rho_1] \\ & + \operatorname*{Tr}_{(2)} [G_{12}A_{12}\rho_2\rho_1 - \rho_1\rho_2 A_{12}G_{12}^{\dagger}] \\ & + \operatorname*{Tr}_{(2)} \Big[G_{12}A_{12}\rho_1\rho_2 G_{12}^{\dagger} \\ & \times (1 - \rho_1)(1 - \rho_2) \frac{1}{E_{12} - H_{12}^{(0)\dagger} - \mathrm{i}\epsilon} \\ & - \frac{1}{E_{12} - H_{12}^{(0)} + \mathrm{i}\epsilon} (1 - \rho_1)(1 - \rho_2) \\ & \times G_{12}A_{12}\rho_1\rho_2 G_{12}^{\dagger} \Big] .\end{aligned} \tag{26}$$

In a forthcoming publication we will discuss the equation in greater detail and show that within the assumptions (weak-coupling limit) it is consistent with energy conservation. To obtain some insight in the physical significance of eq. (26) we rewrite the equation as follows. Define

$$\Sigma_{12} \equiv G_{12}A_{12}\rho_1\rho_2 G_{12}^{\dagger}(1 - \rho_1)(1 - \rho_2) , \tag{27}$$

$$g_{12} \equiv \frac{1}{E_{12} - H_{12}^{(0)} + \mathrm{i}\epsilon} , \tag{28}$$

then

$$\begin{aligned}\mathrm{i}\hbar\partial_t \rho_1 & + [\rho_1, K_1] + [\rho_1, \operatorname*{Tr}_{(2)} \mathrm{Re}\, G_{12}A_{12}\rho_2] \\ & + \operatorname*{Tr}_{(2)} [\mathrm{Re}\, g_{12}\Sigma_{12}^{\dagger} - \Sigma_{12}\, \mathrm{Re}\, g_{12}] \\ & = \operatorname*{Tr}_{(2)} [\mathrm{Im}\, G_{12}A_{12}\rho_2\rho_1 + \rho_1\rho_2 A_{12}\, \mathrm{Im}\, G_{12}] \\ & - \operatorname*{Tr}_{(2)} [\Sigma_{12}\, \mathrm{Im}\, g_{12} + \mathrm{Im}\, g_{12}\Sigma_{12}^{\dagger}] \equiv \mathrm{i}\hbar(\partial_t \rho_1)_{\mathrm{coll}} .\end{aligned} \tag{29}$$

For the discussion of the physical meaning of the individual terms we start with the LHS. The first term determines the time evolution, the second is the kinetic term, the third takes into account the real part of the mean field and the last term is the source of the spreading of the energy spectrum (deviation from a delta function) due to collisions. Setting $\Sigma_{12} = 0$, leads to BHF [15]. The RHS is called the collision term. To obtain its usual form, one has to put ρ diagonal in momentum representation and furthermore the G-matrix on-energy-shell. With these assumptions it follows that:

$$\Sigma_{12}^{\dagger} = \Sigma_{12}\,, \quad \rho_1\rho_2 \operatorname{Im} G_{12} = \operatorname{Im} G_{12}\rho_2\rho_1\,. \tag{30}$$

Note:

$$\operatorname{Im} G_{12} = G_{12}^{\dagger} Q_{12} G_{12} \operatorname{Im} g_{12}\,.$$

Then by approximating $H_{12}^{(0)\dagger} \simeq H_{12}^{(0)}$, the collision term becomes

$$\begin{aligned} i\hbar(\partial_t \rho_1)_{\text{coll}} = 2\pi i \operatorname*{Tr}_{(2)} [&G_{12}A_{12}\rho_1\rho_2 G_{12}^{\dagger} \\ &\times (1-\rho_1)(1-\rho_2)\delta(E_{12} - H_{12}^{(0)}) \\ &- G_{12}^{\dagger}A_{12}(1-\rho_1)(1-\rho_2)G_{12}\rho_1\rho_2 \\ &\times \delta(E_{12} - H_{12}^{(0)})]\,. \end{aligned} \tag{31}$$

This collision operator which consists of a gain and a loss contribution, constitutes together with the LHS of eq. (29) the generalized Boltzmann equation of Kadanoff and Baym [6] (their eq. (9–30)), if one takes the self energy in the so-called "T-approximation". The only difference is in the LHS which in their treatment is only of first order in the gradients.

The well known Uehling–Uhlenbeck equation [11], where the density matrix is assumed to be (almost) diagonal in the momentum representation on both sides of the equation, is now easily obtained. One discards the mean fields U_i and the Pauli operator in the G-matrix equation (25), which then turns into the T-matrix and the resulting equation reads

$$\begin{aligned} i\hbar\partial_t \rho^{(1)}(\boldsymbol{p}_1) = i\pi \int &d^3p_2\, d^3p_1'\, d^3p_2' \\ &\times \{|\langle \boldsymbol{p}_1\boldsymbol{p}_2|T_{12}A_{12}|\boldsymbol{p}_1'\boldsymbol{p}_2'\rangle|^2 \rho^{(1)}(\boldsymbol{p}_1')\rho^{(1)}(\boldsymbol{p}_2') \\ &\times [1-\rho^{(1)}(\boldsymbol{p}_1)][1-\rho^{(1)}(\boldsymbol{p}_2)] \\ &- |\langle \boldsymbol{p}_1'\boldsymbol{p}_2'|T_{12}A_{12}|\boldsymbol{p}_1\boldsymbol{p}_2\rangle|^2 \rho^{(1)}(\boldsymbol{p}_1)\rho^{(1)}(\boldsymbol{p}_2) \\ &\times [1-\rho^{(1)}(\boldsymbol{p}_1')][1-\rho^{(1)}(\boldsymbol{p}_2')]\} \\ &\times \delta(E_{p_1} + E_{p_2} - E_{p_1'} - E_{p_2'})\,. \end{aligned}$$

The step towards the classical Boltzmann equation is of course fully trivial. One simply leaves out the $(1-\rho_1)(1-\rho_2)$ terms (no Pauli blocking) and replaces the quantum mechanical cross sections by classical ones.

Finally we would like to remark that from our discussion is clear that the Uehling–Uhlenbeck equation is merely a very simple extension from classical to quantum mechanics. Indeed it completely neglects the effect of Pauli-blocking and mean field on intermediate states (as displayed by the equation for the G-matrix). Since this has an important effect on the cross section [14,16], one can question its validity.

In conclusion, we derived a quantum kinetic equation, the Brueckner–Boltzmann eq. (26), which is appropriate for intermediate energy nuclear reactions, for it takes account of mean field and two-body collision effects. Furthermore, it is more general than the kinetic equations used up to now in this energy domain [17] because the interaction between the constituents is expressed in a self-consistent way. The use of the Brueckner formalism allows to make contact with microscopic (Dirac–) Brueckner calculations of nuclear matter [14,16] and provides a link between equilibrium and non-equilibrium phenomena.

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